Review of Some Definitions

$\hat{\mathbf{A}} = \text{operator}$

$\psi = \text{state function}$

$$\langle \mathrm{A} \rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\hat{\mathbf{A}}\psi(x,t)dt = \langle \psi | \hat{\mathbf{A}}\psi \rangle = \text{ eigenvalue}$$

if $\hat{\mathbf{A}}$ is a physical operator then A must be a real number.

Hermitian Adjoint

Definition of Hermitian Adjoint

$$\langle \hat{\mathbf{A}}^\dagger \psi_l | \psi_n \rangle = \langle \psi_l | \hat{\mathbf{A}}\psi_n \rangle$$

$$a = A$$

$$\langle a^\dagger \psi_l | \psi_n \rangle = \langle \psi_l | a\psi_n \rangle = a\langle \psi_l | \psi_n \rangle = \langle a^* \psi_l | \psi_n \rangle$$

Example:

$$\hat{\mathbf{D}} = \frac{\partial}{\partial x}$$

$$\hat{\mathbf{D}}^\dagger = ? = -\frac{\partial}{\partial x}$$

$$\langle \psi_l | \hat{\mathbf{D}}\psi_n \rangle = \int_{-\infty}^{\infty} dx\psi_l^* \frac{\partial}{\partial x}\psi_n = \underbrace{\left[\psi_l^* \psi_n\right]_{-\infty}^{\infty}}_{=0} - \int_{-\infty}^{\infty} dx \frac{\partial}{\partial x}\psi_l^* \psi_n = \langle -\hat{\mathbf{D}}\psi_l | \psi_n \rangle$$

$$\therefore \hat{\mathbf{D}}^\dagger = -\hat{\mathbf{D}}$$

Definition:

A is a Hermitian operator (self-adjoint) if and only if A = A†.

$$\hat{\mathbf{A}} = a$$

$$\langle \psi_l | a\psi_n \rangle = \langle a\psi_l | \psi_n \rangle$$

$$\mathrm{A}^\dagger = a^*$$

Now some proofs:

If $\hat{A}=\hat{A}^\dagger$ and $\hat{B}=\hat{B}^\dagger$

$$\hat{A}\hat{B}\overset{?}{=}\left(\hat{A}\hat{B}\right)^\dagger=\hat{B}^\dagger\hat{A}^\dagger$$

Dr. Shen gave us some time in class to prove that

$$\left(\hat{A}\hat{B}\right)^\dagger=\hat{B}^\dagger\hat{A}^\dagger$$

Proof:

$$\left\langle\left(\hat{A}\hat{B}\right)^\dagger\psi_l\middle|\psi_n\right\rangle=\left\langle\psi_l\middle|\left(\hat{A}\hat{B}\right)\psi_n\right\rangle=\left\langle\hat{A}^\dagger\psi_l\middle|\left(\hat{B}\right)\psi_n\right\rangle=\left\langle\hat{B}^\dagger\hat{A}^\dagger\psi_l\middle|\psi_n\right\rangle$$

$$\therefore\left(\hat{A}\hat{B}\right)^\dagger=\hat{B}^\dagger\hat{A}^\dagger=\hat{B}\hat{A}$$

Momentum Operator:

$$\hat{p}=-i\hbar\frac{\partial}{\partial x}$$

$$\hat{p}\overset{?}{=}\hat{p}^\dagger$$

From the definition of a Hermitian operator:

$$\left\langle\psi_l\,|\,\hat{p}\psi_n\right\rangle=\left\langle\psi_l\middle|\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_n\right\rangle=\int_{-\infty}^{\infty}\psi_l^*\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_n dx$$

$$=-i\hbar\int_{-\infty}^{\infty}\psi_l^*\left(\frac{\partial}{\partial x}\right)\psi_n dx=-i\hbar\underbrace{\left[\psi_l^*\psi_n\right]_{-\infty}^{\infty}}_{=0}+\int_{-\infty}^{\infty}i\hbar\frac{\partial}{\partial x}\psi_l^*\psi_n dx$$

$$=\int_{-\infty}^{\infty}\left(-i\hbar\frac{\partial}{\partial x}\psi_l\right)^*\psi_n dx=\int_{-\infty}^{\infty}\left(\hat{p}\psi_l\right)^*\psi_n dx$$

$$=\left\langle\hat{p}\psi_l\middle|\psi_n\right\rangle$$

$$\therefore\ \hat{p}^\dagger=\hat{p}$$

Free Particle Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V$$

$$\left(\hat{p}\hat{p}\right)^\dagger = \hat{p}\hat{p} + V \leftarrow \text{if Potential is a real number}$$

$\therefore$ the Hamiltonian is a Hermitian operator

$$\langle A\rangle^* = \left[\int_{-\infty}^{\infty} \psi^* A\psi\, dx\right]^* = \int_{-\infty}^{\infty} \psi\left[A\psi\right]^* dx = \langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle = \langle A\rangle$$

For operator – eigenvalue equation – prove that wavefunctions are orthogonal (perpendicular)

$$\hat{A}\psi_n = a_n\psi_n$$

Prove that $\langle\psi_n|\psi_l\rangle = 0$ when $n \neq l$

$$\left|\hat{A}\psi_n\right\rangle = a_n\left|\psi_n\right\rangle$$

$$\langle A\rangle = \left\langle\psi_n\middle|\hat{A}\psi_n\right\rangle = \langle\psi_n|a_n\psi_n\rangle = a_n\underbrace{\langle\psi_n|\psi_n\rangle}_{=1} = a_n$$

$$\left\langle\psi_l\middle|\hat{A}\psi_n\right\rangle = \langle\psi_l|a_n\psi_n\rangle = a_n\langle\psi_l|\psi_n\rangle$$

$$\left\langle\hat{A}\psi_l\middle|\psi_n\right\rangle = a_l^*\langle\psi_l|\psi_n\rangle = a_l$$

$$\left(a_l - a_n\right)\langle\psi_l|\psi_n\rangle = 0$$

but $\left(a_l - a_n\right) \neq 0$

$$\therefore \langle\psi_l|\psi_n\rangle = 0$$

☼ Homework: 5.12, 5.13, 6.19 and

If $\hat{C}\psi = \psi^*$

is $\hat{C}$ Hermitian?

Find $\hat{C} = \hat{C}^\dagger$

$$\langle C\rangle = \int\psi^*\left(\hat{C}\psi\right)dx = \int\psi^*\psi^*\,dx = ?$$